Non-Linear Reaction-Diffusion Process in a Thin Membrane and Homotopy Analysis Method

V. Ananthaswamy¹, A. Eswari², L. Rajendran³

^{1,3} Department of Mathematics, The Madura College (Autonomous), Madurai, Tamil nadu, India

²Department of Mathematics, K.L.N. College of Engineering, Madurai, Tamil nadu, India

¹ananthu9777@rediffmail.com; ²alagueswari@gmail.com; ³raj_sms@rediffmail.com

Abstract

The system of non linear reaction-diffusion process in thin membrane describing steady state of chemical reactions that involves three species is discussed. The equations are coupled by the non-linear reaction terms with mixed boundary conditions. A closed form of an analytical expression of concentrations for the full range of enzyme activities has been derived using Homotopy analysis method. A simple form of an approximate analytical expression of concentrations in terms of dimensionless parameter λ is also reported. These approximate results are compared with the numerical results. A good agreement with simulation data is noted.

Keywords

Non-Llinear Reaction-Diffusion Equations; Enzyme Mathematical Modeling; Thin Membrane; Homotopy Analysis Method; Matlab Program

Introduction

We consider a diffusion controlled chemical reaction between two species A and B to form a product, according to the reaction mechanism $2A+B \rightarrow product$. This reaction takes place within a thin membrane between 'tanks' with abundant supplies of A to the left of B to the right of the membrane. We model the transport inside the membrane as diffusive, thus the model will be given by a system of non-linear reaction-diffusion equations that are coupled with the non-linear reaction terms. The reaction path consists of a coupled pair of rapid irreversible simple reaction mechanism [Ariel (2010)].

$$A + B \xrightarrow{\lambda} C,$$

$$A + C \xrightarrow{\mu} product$$
(1)

where λ and μ denote the binary reaction rates.

Seidman et. al (1997 and 2005) and Kalacheve et. al. (2003) provided the rigorous singular perturbation analysis for the steady-state problem. corresponding non-steady state system of this problem has been considered by Haario Seidman (1994), for the complex boundary conditions, to describe reactions in the film model for a gas/liquid interface. Also the steady state problem has many important applications, in chemical engineering modeling. Recently, Butuzov et al. (1999 and 2007) have obtained some related problems of exchange of stabilities using different techniques (upper and lower solutions). However, to the best of author's knowledge, no general analytical results of substrate concentration for all values of dimensionless parameter λ have been published. The purpose of this communication is to derive approximate analytical expressions for the steady-state concentrations for all values of λ using Homotopy analysis method.

Mathematical Formulation of the Problems

The governing non-linear reaction diffusion equation in a thin membrane is expressed in the following non-dimensional format [Ariel (2010)]:

$$u_{xx} = \lambda uv + uw \tag{2}$$

$$v_{xx} = \lambda uv \tag{3}$$

$$w_{yy} = uw - \lambda uv \tag{4}$$

where u(x), v(x) and w(x) denote the concentrations of the chemical species A, B and C respectively. The diffusion coefficients of three species are considered to have an equal diffusion coefficient which is equal to 1. We assume that the specie A is supplied with a given fixed concentration $\alpha > 0$ at x = 0, and the specie B with $\beta > 0$ at x = 1. Boundary conditions are

$$u = \alpha$$
; $v_x = 0$; $w = \gamma$ at $x = 0$ (5)

$$u_x = 0$$
; $v = \beta$; $w_x = 0$ at $x = 1$ (6)

Since the appearance of the large factor λ is much greater than 1 in one of the terms in each reaction-diffusion equations (2)-(4) the equations have singularly perturbed problems [Ariel (2010)].

Solution of Boundary Value Problem Using Homotopy Analysis Method (HAM)

Liao (1992, 1995, 2003, 2004, 2010 and 2012) proposed a powerful analytical method for non-linear problems, namely the Homotopy analysis method. This method provides an analytical solution in terms of an infinite power series. However, there is a practical need to evaluate this solution and to obtain numerical values from the infinite power series. In order to investigate the accuracy of the Homotopy analysis method (HAM) solution with a finite number of terms, the differential equations in the system were solved. The Homotopy analysis method [Liao (1992, 1995, 2003, 2004, 2010, 2012), Eswari et.al (2010) and Jafari et. al (2009)] is a preferred technique comparing another perturbation method.

Homotopy perturbation method [Chowdhury et. al (2007), Eswari et.al (2010), Ghori et. al (2007), Coyle et. al (1986), Ozis et. al (2007), Madden et. al (2003)] is a special case of Homotopy analysis method. Different from all reported perturbation and non perturbative techniques, the Homotopy analysis method itself provides us with a convenient way to control and adjust the convergence region and approximation series, when necessary. speaking, the Homotopy analysis method has the following advantages: itt is valid even if a given nonlinear problem does not contain any small/large parameter at all; it can be employed to efficiently approximate a nonlinear problem by choosing different sets of base functions. The Homotopy analysis method contains the auxiliary parameter hwhich provides us with a simple way to adjust and control the convergence region of solution series. Using this method, we can obtain the following solution to (2) - (6) (see Appendix B).

$$u(x) = \alpha + h\alpha \left[\lambda \beta + \gamma\right] \left(x - \frac{x^2}{2}\right) \tag{7}$$

$$v(x) = \beta + \left(\frac{h\lambda\alpha\beta(1-x^2)}{2}\right)$$
 (8)

and

$$w(x) = h\alpha(\gamma - \lambda\beta)x + \left(\frac{h\alpha(\lambda\beta - \alpha\gamma)x^2}{2}\right)$$
 (9)

The equations (7)-(9) represent the new analytical expression of concentration of species for all values of dimensionless parameter. The reaction rate q is given by

$$q = \lambda uv = \lambda \left\{ \left[\alpha + h\alpha \left[\lambda \beta + \gamma \right] \left(x - \frac{x^2}{2} \right) \right] \right\}$$

$$\left[\beta + \left(\frac{h\lambda \alpha \beta (1 - x^2)}{2} \right) \right]$$
(10)

Numerical Simulation

In order to find reveal the accuracy of our analytical method, the non-linear differential eqns. (2)-(4) are also solved by numerical methods. The function *bvp4c* in Matlab software which is a function of solving two-point boundary value problems (TPBVPs) for ordinary differential equations is used to solve these equations numerically. Our analytical result is compared with numerical solution and it gives a satisfactory agreement (See figures (1-3)). The Matlab program is also given in Appendix D.

Results and Discussions

Fig. 1 represents the normalized steady-state concentration u(x)different values for dimensionless parameter $\lambda = 0.1, 0.5, 1, 3$ and 5. From this figure, it is evident that the values of the decreases when dimensionless concentration x = 1. **Fig. 2** shows the parameter λ increases to normalized steady-state concentration v(x) versus the dimensionless distance x for various values of dimensionless parameter λ . From this figure, it is obvious that the values of the concentration increases when dimensionless parameter λ decreases to x = 0. The normalized steady-state concentration w(x)versus the dimensionless distance x for various values of dimensionless parameter λ is plotted in the **Fig. 3**. From this figure, it is inferred that the value of the concentration will increase, when the diffusion parameter λ increases. Fig.4 shows the normalized steady state concentrations u(x), v(x) and w(x) for some fixed value of $\lambda = 5$. From this figure it is observed that the concentration u(x) of species A from its initial value, where the concentrations v(x) of the species B and w(x) of the species C increase from its initial

values.

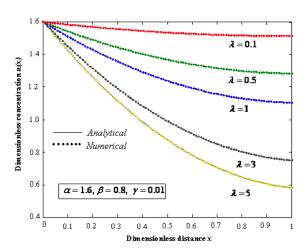


Fig. 1 Normalized steady-state concentration u(x) versus the dimensionless distance x. The concentrations were computed using (7) for various values of the dimensionless parameter λ and h=-0.2.

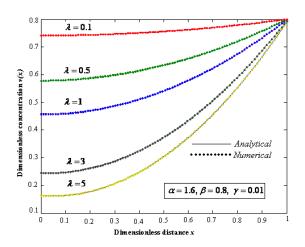


Fig. 2 Normalized steady-state concentration v(x) versus the dimensionless distance x . The concentrations were computed using (8) for various values of the dimensionless parameter λ and h=-0.2.

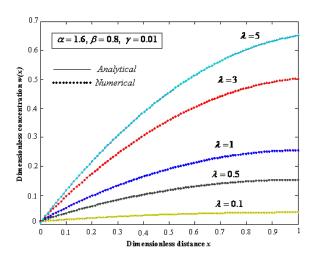


Fig. 3 Normalized steady-state concentration w(x) versus the dimensionless distance x . The concentrations were computed using (9) for various values of the dimensionless parameter λ and h=-0.2.

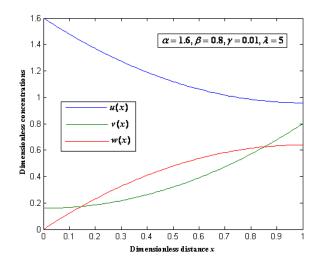


Fig. 4. Normalized steady-state concentration u(x), v(x) and w(x) versus the dimensionless distanc x . The concentrations were computed using (7) - (9) and for the fixed value of the dimensionless parameter $\lambda=5$ and h=-0.2.

Figs. 5-7 shows the dimensionless reaction rate q using for various values of λ . Thus, it is concluded that there is a simultaneous increase in the values of the reaction rate as well as in λ for the fixed value of α , β and γ . The optimum value of h can be obtained using h curve which is given in the **Figures 8-9**.

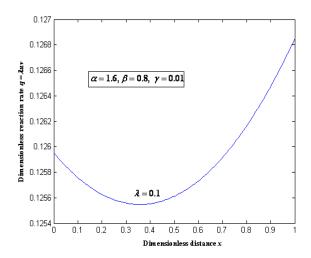


Fig. 5 Dimensionless reaction rate versus the dimensionless distance x using (10) for the value of the dimensionless parameter $\lambda=0.1$ when $\alpha=1.6,~\beta=0.8,~\gamma=0.01$ and h=-0.2.

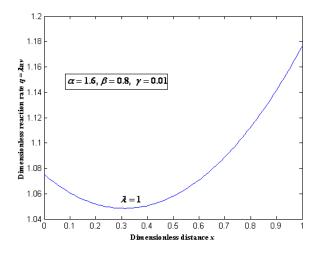


Fig. 6 Dimensionless reaction rate versus the dimensionless distance x using (10) for the value of the dimensionless parameter $\lambda=1$, when $\alpha=1.6$, $\beta=0.8$, $\gamma=0.01$ and h=-0.2.

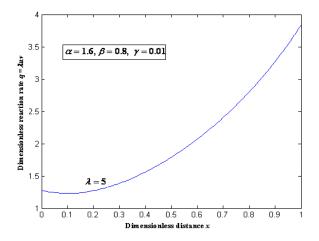


Fig. 7 Dimensionless reaction rate versus the dimensionless distance x using (10) for the value of the dimensionless parameter $\lambda=5$, when $\alpha=1.6$, $\beta=0.8$, $\gamma=0.01$ and h=-0.2.

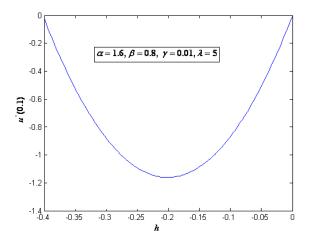


Fig. 8 The $\,h$ curve to indicate the convergence region $\,u\,$ (0.1) for when $\,\alpha=1.6,\,\,\,\beta=0.8,\,\gamma=0.01\,$ and $\,\lambda=5.$

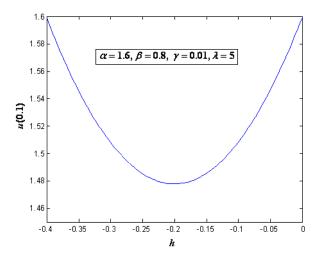


Fig. 9 The h curve to indicate the convergence region u(0.1) for when $\alpha=1.6$, $\beta=0.8$, $\gamma=0.01$ and $\lambda=5$.

Conclusion

The system of time independent reaction-diffusion equation coupled through the non linear reaction terms in thin membrane has been solved analytically and numerically. Analytical expressions of the concentrations of species are derived by using the Homotopy analysis method. The primary result of this work is simple and approximate expressions of the concentrations for all values of the dimensionless parameter λ . This analytical result will be useful to analyze the behavior of the internal layers. This method is an extremely simple and it is also a promising method to solve other non-linear equations. This method can be easily extended to find the solution of all other non-linear equations.

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Appendix A: Basic Concept of Homotopy Analysis Method (HAM)

Consider the following differential equation:

$$N[u(t)] = 0 \tag{A.1}$$

Where N is a nonlinear operator, t denotes an

independent variable, u(t) is an unknown function. For simplicity, we ignore all boundary or initial conditions, which can be treated in the similar way. By means of generalizing the conventional Homotopy method, Liao (2012) constructed the so-called zero-order deformation equation as:

$$(1-p)L[\varphi(t;p) - u_0(t)] = phH(t)N[\varphi(t;p)]$$
 (A.2)

where $p \in [0,1]$ is the embedding parameter, $h \neq 0$ is a nonzero auxiliary parameter, $H(t) \neq 0$ is an auxiliary

function, L an auxiliary linear operator, u_0 (t) is an initial guess of u(t), $\varphi(t:p)$ is an unknown function. It is important to note that one has great freedom to choose auxiliary unknowns in HAM. Obviously, when p=0 and p=1, it holds:

$$\varphi(t;0) = u_0(t) \text{ and } \varphi(t;1) = u(t)$$
 (A.3)

respectively. Thus, as p increases from 0 to 1, the solution $\varphi(t;p)$ varies from the initial guess $u_0(t)$ to the solution u(t). Expanding $\varphi(t;p)$ in Taylor series with respect to p, we have:

$$\varphi(t;p) = u_0(t) + \sum_{m=1}^{+\infty} u_m(t) p^m$$
(A.4)

where

$$u_m(t) = \frac{1}{m!} \frac{\partial^m \varphi(t; p)}{\partial p^m} \Big|_{p=0}$$
 (A.5)

If the auxiliary linear operator, the initial guess, the auxiliary parameter h, and the auxiliary function are so properly chosen, the series (A.4) converges at p =1 then we have:

$$u(t) = u_0(t) + \sum_{m=1}^{+\infty} u_m(t)$$
 (A.6)

Differentiating (A.2) for m times with respect to the embedding parameter p, and then setting p = 0 and finally dividing them by m!, we will have the so-called mth -order deformation equation as:

$$L[u_m - \chi_m u_{m-1}] = hH(t) \mathfrak{R}_m(\vec{u}_{m-1}) \tag{A.7}$$

where

$$\mathfrak{R}_{m}(\vec{u}_{m-1}) = \frac{1}{(m-1)!} \frac{\partial^{m-1} N[\varphi(t;p)]}{\partial p^{m-1}}$$
(A.8)

And

$$\chi_m = \begin{cases} 0, & m \le 1, \\ 1, & m > 1. \end{cases}$$
 (A.9)

Applying L^{-1} on both side of equation (A7), we get

$$u_m(t) = \chi_m u_{m-1}(t) + hL^{-1}[H(t)\mathfrak{R}_m(u_{m-1})]$$
(A10)

In this way, it is easily to obtain u_m for $m \ge 1$, at M^{th} order, we have

$$u(t) = \sum_{m=0}^{M} u_m(t)$$
 (A.11)

When $M \to +\infty$, we get an accurate approximation of the original equation (A.1). For the convergence of the above method we refer the reader to Liao [20]. If equation (A.1) admits unique solution, then this method will produce the unique solution.

Appendix B: Solution of Non-linear Equations (2) to (6) Using HAM

In this Appendix, we indicate how (7) to (9) in this paper are derived. To find the solution of (2), (3) and (4), it can be simplified to [Ariel (2010)]

$$\frac{d^2u}{dx^2} - \lambda uv - uw = 0 ag{B.1}$$

$$\frac{d^2v}{dx^2} - \lambda uv = 0 ag{B.2}$$

$$\frac{d^2w}{dx^2} - uw + \lambda uv = 0 ag{B.3}$$

Now the boundary conditions becomes

$$x=0$$
, $u=\alpha$, $\frac{dv}{dx}=0$, $w=\gamma$ (B.4)

$$x = 1$$
, $\frac{du}{dx} = 0$, $v = \beta$, $\frac{dw}{dx} = 0$ (B.5)

We construct the Homotopy as follows

$$(1-p)\left[\frac{d^2u}{dx^2}\right] = hp\left[\frac{d^2u}{dx^2} - \lambda uv - uw\right]$$
 (B.6)

$$(1-p)\left[\frac{d^2v}{dx^2}\right] = hp\left[\frac{d^2v}{dx^2} - \lambda uv\right]$$
 (B.7)

$$(1-p)\left[\frac{d^2w}{dx^2}\right] = hp\left[\frac{d^2w}{dx^2} + \lambda uv - uw\right]$$
 (B.8)

The approximate solution of (B.1) and (B.2) and (B.3) is,

$$u = u_0 + pu_1 + p^2 u_2 + \dots$$
 (B.9)

$$v = v_0 + pv_1 + p^2v_2 + \dots$$
 (B.10)

$$w = w_0 + pw_1 + p^2w_2 + \dots$$
 (B.11)

The initial approximations are as follows

$$u_0(0) = \alpha \text{ and } u_0(1) = 0$$
 (B.12)

$$u_i(0) = 0$$
 and $u_i(1) = 0$, $i = 1,2...$ (B.13)

$$v_0'(0) = 0$$
 and $v_0(1) = \beta$ (B.14)

$$v_i(0) = 0$$
 and $v_i(1) = 0$, $i = 1,2...$ (B.15)

$$w_0(0) = \gamma \text{ and } w_0(1) = 0$$
 (B.16)

$$w_i(0) = 0$$
 and $w_i(1) = 0, i = 1,2...$ (B.17)

Substituting (B.9) to (B.11) into (B.6) to (B.8) we have

$$(1-p)\left[\frac{d^{2}(u_{0}+pu_{1}+...)}{dr^{2}}\right]$$

$$=hp\begin{bmatrix} \frac{d^{2}(u_{0}+pu_{1}+...)}{dx^{2}}\\ -\lambda(u_{0}+pu_{1}+....)(v_{0}+pv_{1}+....)\\ -(u_{0}+pu_{1}+....)(w_{0}+pw_{1}+....) \end{bmatrix}$$
(B.18)

$$(1-p)\left[\frac{d^{2}(v_{0}+pv_{1}+..)}{dx^{2}}\right]$$

$$=hp\left[\frac{d^{2}(v_{0}+pv_{1}+..)}{dx^{2}}\right]$$

$$-\lambda(u_{0}+pu_{1}+...)(v_{0}+pv_{1}+....)$$
(B.19)

$$(1-p) \left[\frac{d^{2}(w_{0} + pw_{1} +)}{dx^{2}} \right]$$

$$= hp \left[\frac{d^{2}(w_{0} + pw_{1} +)}{dx^{2}} + \lambda(u_{0} + pu_{1} +)(v_{0} + pv_{1} + ...)}{-(u_{0} + pu_{1} +)(w_{0} + pw_{1} + ...)} \right]$$
(B.20)

Comparing the coefficients of like powers of p in (B.18) we get

$$p^{0}: \frac{d^{2}u_{0}}{dx^{2}} = 0 {(B.21)}$$

$$p^{1}: \frac{d^{2}u_{1}}{dx^{2}} - (h+1) \left[\frac{d^{2}u_{0}}{dx^{2}} \right] + h\lambda u_{0}v_{0} + hu_{0}w_{0} = 0$$
 (B.22)

Comparing the coefficients of like powers of p in (B.19) we obtain.

$$p^{0}: \frac{d^{2}v_{0}}{dx^{2}} = 0 {(B.23)}$$

$$p^{1}: \frac{d^{2}v_{1}}{dx^{2}} - (h+1) \left[\frac{d^{2}v_{0}}{dx^{2}} \right] + h\lambda u_{0}v_{0} = 0$$
 (B.24)

Comparing the coefficients of like powers of p in (B.20) we have

$$p^{0}: \frac{d^{2}w_{0}}{dx^{2}} = 0 {(B.25)}$$

$$p^{1}: \frac{d^{2}u_{1}}{dx^{2}} - (h+1) \left[\frac{d^{2}w_{0}}{dx^{2}} \right] + hu_{0}w_{0} - h\lambda u_{0}v_{0} = 0 \quad (B.26)$$

Solving (B.21) to (B.26) and using the boundary conditions (B.12) to (B.17), we can obtain the following results:

$$u_0 = \alpha, \quad u_1 = h\alpha \left[\lambda \beta + \gamma\right] x, \quad v_0 = \beta,$$

$$v_1 = \left(\frac{h\lambda \alpha \beta (1 - x^2)}{2}\right)$$
(B.27)

$$w_0 = 0, \ w_1 = h\alpha(\gamma - \lambda\beta)x + \left(\frac{h\alpha(\lambda\beta - \alpha\gamma)x^2}{2}\right)$$
 (B.28)

According to the HPM, we can conclude that

$$u = \lim_{n \to 1} u(x) = u_0 + u_1 \tag{B.29}$$

$$v = \lim_{p \to 1} v(x) = v_0 + v_1 \tag{B.30}$$

$$w = \lim_{p \to 1} w(x) = w_0 + w_1 \tag{B.31}$$

After putting (B.27) and (B.28) into (B.29) to (B.31), we obtain (7) - (9) in the text.

Appendix C: Determining the Region of h for Validity

The analytical solution should converge. It should be noted that the auxiliary parameter h controls the convergence and accuracy of the solution series. The analytical solution represented by (7) contains the auxiliary parameter h which gives the convergence region and rate of approximation for the Homotopy analysis method. In order to define region such that the solution series is independent of h, a multiple of h curves are plotted. The region where the concentration u(x) and u'(x) versus h is a horizontal line known as the convergence region for the corresponding function. The common region among u(x) and its derivatives are known as the over all convergence region. To study the influence of h on the convergence of solution, h curves of u(0.1) and u'(0.1) are plotted in Fig. (7) and (8) respectively for $\alpha = 1.6$, $\beta = 0.8$, $\gamma = 0.01$ and $\lambda = 5$. These figures clearly indicate that the valid region of h is about (-0.4 to -0.05). Similarly we can find the value of the convergence control parameter h for different values of constant parameters.

Appendix D: Matlab Program to Find the Numerical Solution of Non-linear Equations (2) to (6):

```
function pdex4
m = 0;
x = linspace(0,1);
t=linspace(0,100000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u1 = sol(:,:,1);
u2 = sol(:,:,2);
u3=sol(:,:,3);
figure
plot(x,u1(end,:))
title('u1(x,t)')
xlabel('Distance x')
ylabel('u1(x,2)')
%_____
Figure
plot(x,u2(end,:))
title('u2(x,t)')
xlabel('Distance x')
vlabel('u2(x,2)')
Figure
plot(x,u3(end,:))
title('Solution at t = 2')
xlabel('Distance x')
ylabel('u3(x,2)')
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = [1; 1; 1];
f = [1; 1; 1] * DuDx;
y = u(1) * u(2);
y1=u(1)*u(3);
```

```
alpha=1.6;
gamma=0.01;
beta=0.8;
lamta=5; % parameters
F = (-lamta*y-y1);
F1=(-lamta*y);
                   % non linear terms
F2=(lamta*y-y1);
s=[F;F1;F2];
Function u0 = pdex4ic(x);
%create a initial conditions
u0 = [0; 1; 0];
function[pl,ql,pr,qr]=pdex4bc(xl,u1,xr,ur,t)
 %create a boundary conditions
pl = [u1(1)-1.6; 0; u1(3)-0.01];
ql = [0; 1; 0];
pr = [0; ur(2)-0.8; 0];
qr = [1; 0; 1];
```

Appendix E: Nomenclature

Symbol	Meaning
и	Concentration of the chemical species A
v	Concentration of the chemical species <i>B</i>
w	Concentration of the chemical species C
λ	Dimensionless parameter
х	Dimensionless distance
α	Fixed concentration of the species A
β	Fixed concentration of the species <i>B</i>
γ	Fixed concentration of the species <i>C</i>
q	Dimensionless reaction rate

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Author Introduction



Mr. V. Ananthaswamy received his M.Sc. Mathematics degree from The Madura College (Autonomous), Madurai-625011, Tamil Nadu, India during 2000. He has received his M. Phil degree in Mathematics from Madurai Kamaraj University, Madurai, Tamil Nadu, India during 2002. Also he is

doing his Ph.D, in "Some Boundary value Problems in Reaction Diffusion Processes" at Madurai Kamaraj University, Madurai, under the guidance of Dr. L. Rajendran. He has 12 years and six months of teaching experiences for Engineering College, Arts College and Deemed University and 3 years of research experience. At present he is working as Assistant Professor in Mathematics, The Madura College (Autonomous), Madurai-625 011 from 2008 onwards. He has published five articles in peer-reviewed journals. present research interest includes: Mathematical modeling based on differential equations and asymptotic approximations, analysis of system of non-linear reaction diffusion equations in physical sciences. Also, he has participated and presented research papers in National Conferences.



Ms. A. Eswari received her M.Sc (2005) and M.Phil (2006) in Mathematics from Madura College and Mannar Thirumalai Naicker College, Madurai, Tamilnadu, India. At present, She is working as a Associate Professor in Mathematics Department. at K.L.N. College of Engineering, Pottapalayam, Sivagangai District, Tamilnadu, India.

Also, she is doing her Ph.D in Mathematical modelling at Manonmaniam Sundaranar University, Tirunelveli under the guidance of Dr. L. Rajendran, Department of Mathematics, The Madura College, Madurai. Her present research interest include: Mathematical modelling,

Analytical solution of system of nonlinear reaction diffusion processes in biosensor, variational iteration, Homotopy perturbation and numerical methods. She has published 15 papers in International Journals, 2 papers have been communicated in International Journals and one paper has been accepted in Book for publication. Also, She has participated and presented research papers in International and National Conferences.



Dr. L. Rajendran received his M.Sc. in Mathematics in 1981 from Presidency College, Chennai, TN, India. He obtained his Ph.D. in Applied Mathematics from Alagappa University, Karaikudi, TN, India during 2000. At present, he is an Assistant Professor in Matheatics at The Masdura College(Autonomous), Madurai, TN, India. Before this position

(1986–2007), he was working as a Post Graduate Assistant in Mathematics at SMSV Higher Secondary School, Karaikudi, TN, India. He has 20 years teaching experience and 15 years research experience. He has authored and coauthor over 100 research publications including about 70 scholarly articles in peer-reviewed journals. He visited institute fur Organische Chemie, Universitry at Tubingen, D- 72076 Tubingen, Germany in year 2003 under INSA and DFG Postdoctoral Research Fellowship. Currently he has three research projects from DST, CSIR and UGC. His current research interests include mathematical and computational modeling of electrochemical biosensor.